Table IS: The BODC calculated using the cc-pVTZ basis and CASSCF wavefunction using the 6,2 active space. The coordinates are in degrees and angstroms, and the energies are in Hartree atomic units.

Theta	R1	R2	CASSCF Energy	BODC
90.0	0.825	0.875	-76.14115013511955	0.00277892186022
100.0	0.825	0.875	-76.14942981432102	0.00277130282264
110.0	0.825	0.875	-76.15163441222333	0.00276184734085
120.0	0.825	0.875	-76.14882372121596	0.00275041653013
130.0	0.825	0.875	-76.14221823188289	0.00273738527118
90.0	0.825	0.925	-76.14963127674271	0.00277418880383
100.0	0.825	0.925	-76.15708619012791	0.00276636611455
110.0	0.825	0.925	-76.15862276832705	0.00275690483043
120.0	0.825	0.925	-76.15525324668290	0.00274559984994
130.0	0.825	0.925	-76.14815844502559	0.00273275806462
140.0	0.825	0.925	-76.13874042542503	0.00271914464710
80.0	0.825	0.975	-76.13856260595357	0.00277887976994
90.0	0.825	0.975	-76.15184075002600	0.00277146102481
100.0	0.825	0.975	-76.15847822356267	0.00276348651687
110.0	0.825	0.975	-76.15935674848247	0.00275408676414
120.0	0.825	0.975	-76.15543929024567	0.00274299706597
130.0	0.825	0.975	-76.14786338552064	0.00273045994838
140.0	0.825	0.975	-76.13799714418974	0.00271717772521
90.0	0.825	1.025	-76.14957250378279	0.00277048163383
100.0	0.825	1.025	-76.15540803802051	0.00276242078860
110.0	0.825	1.025	-76.15564597617411	0.00275316101853
120.0	0.825	1.025	-76.15119869577241	0.00274238687992
130.0	0.825	1.025	-76.14315613659727	0.00273030198196
90.0	0.825	1.075	-76.14414263351124	0.00277106699768
100.0	0.825	1.075	-76.14919875199355	0.00276298665111
110.0	0.825	1.075	-76.14882023437588	0.00275395902750
120.0	0.825	1.075	-76.14386756013863	0.00274363174893
80.0	0.875	0.875	-76.14390754627935	0.00277852409859
90.0	0.875	0.875	-76.15832700084385	0.00277159825471
100.0	0.875	0.875	-76.16585713346096	0.00276382765737
110.0	0.875	0.875	-76.16744798498848	0.00275439334611
120.0	0.875	0.875	-76.16411861790129	0.00274309063537
130.0	0.875	0.875	-76.15705666946307	0.00273022339102
140.0	0.875	0.875	-76.14767020076673	0.00271655241456
150.0	0.875	0.875	-76.13759285485969	0.00270325013300
80.0	0.875	0.925	-76.15330582503677	0.00277390254403
90.0	0.875	0.925	-76.16677565110659	0.00276662190663
100.0	0.875	0.925	-76.17355071102428	0.00275873625317
110.0	0.875	0.925	-76.17452759117209	0.00274937583324
120.0	0.875	0.925	-76.17068197153031	0.00273827503285
130.0	0.875	0.925	-76.16316462029232	0.00272567543693
140.0	0.875	0.925	-76.15335548839066	0.00271226030211
150.0	0.875	0.925	-76.14287827114632	0.00269913515424
80.0	0.875	0.975	-76.15644091158823	0.00277127177078
90.0	0.875	0.975	-76.16895803760730	0.00276366731576
100.0	0.875	0.975	-76.17498167319660	0.00275571502046
110.0	0.875	0.975	-76.17535258479464	0.00274649189852
120.0	0.875	0.975	-76.17100083917940	0.00273568057650
130.0	0.875	0.975	-76.16303564250589	0.00272347056493
140.0	0.875	0.975	-76.15280234944308	0.00271046894160
150.0	0.875	0.975	-76.14190974081207	0.00269771055200
80.0	0.875	1.025	-76.15509753924621	0.00277035554977
90.0	0.875	1.025	-76.16666964700627	0.00276247101563
100.0	0.875	1.025	-76.17195342500500	0.00275451079816
110.0	0.875	1.025	-76.17173352948647	0.00274550103927
120.0	0.875	1.025	-76.16689243032747	0.00273508547666
130.0	0.875	1.025	-76.15849258961346	0.00272341110514
140.0	0.875	1.025	-76.14783761518271	0.00271101610819
80.0	0.875	1.075	-76.15058372121138	0.00277094640111
90.0	0.875	1.075	-76.16122728878889	0.00276283461232

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110.0	0.875	1.075	-76.16500055480294	0.00274622813213
120.0	0.875	1.075	-76.15969275922154	0.00273633727046
130.0	0.875	1.075	-76.15087655775628	0.00272537861633
140.0	0.875	1.075	-76.13980609017912	0.00271382976840
80.0	0.925	0.925	-76.16258794066280	0.00276898438086
90.0	0.925	0.925	-76.17519386269728	0.00276143576048
100.0	0.925	0.925	-76.18128120383014	0.00275351574147
110.0	0.925	0.925	-76.18169719318453	0.00274430309024
120.0	0.925	0.925	-76.17737788405216	0.00273347926513
130.0	0.925	0.925	-76.16943896050887	0.00272122949834
140.0	0.925	0.925	-76.15923175556149	0.00270815339143
150.0	0.925	0.925	-76.14836863962765	0.00269528002571
80.0	0.925	0.975	-76.16561576979007	0.00276608198179
90.0	0.925	0.975	-76.17735046311270	0.00275829241465
100.0	0.925	0.975	-76.18275083460196	0.00275038045608
110.0	0.925	0.975	-76.18261243018507	0.00274137514870
120.0	0.925	0.975	-76.17782884166309	0.00273091625543
130.0	0.925	0.975	-76.16947516232236	0.00271914060467
140.0	0.925	0.975	-76.15886721221636	0.00270656956205
150.0	0.925	0.975	-76.14760082657344	0.00269415122232
80.0	0.925	1.025	-76.16417617928026	0.00276490499536
90.0	0.925	1.025	-76.17504257015675	0.00275691644876
100.0	0.925	1.025	-76.17976428546407	0.00274906730151
110.0	0.925	1.025	-76.17908468354618	0.00274034333513
120.0	0.925	1.025	-76.17385228604283	0.00273035481896
130.0	0.925	1.025	-76.16509587418733	0.00271920358295
140.0	0.925	1.025	-76.15408842346547	0.00270733783423
150.0	0.925	1.025	-76.14240284393829	0.00269563184045
80.0	0.925	1.075	-76.15957816047012	0.00276523451813
90.0	0.925	1.075	-76.16958781043817	0.00275709903778
100.0	0.925	1.075	-76.17364591590635	0.00274937722821
110.0	0.925	1.075	-76.17244435925552	0.00274102372079
120.0	0.925	1.075	-76.16678411623295	0.00273163606011
130.0	0.925	1.075	-76.15764192462136	0.00272129078961
140.0	0.925	1.075	-76.14624020465315	0.00271037903340
80.0	0.975	0.975	-76.16854341090082	0.00276293694936
90.0	0.975	0.975	-76.17948514350110	0.00275498301725
100.0	0.975	0.975	-76.18426082782565	0.00274714766535
110.0	0.975	0.975	-76.18361845175636	0.00273841582636
120.0	0.975	0.975	-76.17841174818436	0.00272839493708
130.0	0.975	0.975	-76.16967571153653	0.00271718169787
140.0	0.975	0.975	-76.15868962087865	0.00270521447520
150.0	0.975	0.975	-76.14703090463263	0.00269335782182
80.0	0.975	1.025	-76.16701296056587	0.00276153331571
90.0	0.975	1.025	-76.17716084118669	0.00275345320735
100.0	0.975	1.025	-76.18131754468875	0.00274574399257
110.0	0.975	1.025	-76.18018272851653	0.00273735649163
120.0	0.975	1.025	-76.17456716392901	0.00272788004617
130.0	0.975	1.025	-76.16545981390631	0.00271738098246
140.0	0.975	1.025	-76.15409612277264	0.00270622772294
150.0	0.975	1.025	-76.14202836922681	0.00269521122573
80.0	0.975	1.075	-76.16233458752073	0.00276163930092
90.0	0.975	1.075	-76.17169604926923	0.00275348431807
100.0	0.975	1.075	-76.17524592453881	0.00274596204370
110.0	0.975	1.075	-76.17363588073351	0.00273800512793
120.0	0.975	1.075	-76.16763087812815	0.00272920261751
130.0	0.975	1.075	-76.15816814117213	0.00271960139172
140.0	0.975	1.075	-76.14643172097823	0.00270952108521
80.0	1.025	1.025	-76.16539927787099	0.00275992273918
90.0	1.025	1.025	-76.17482481309381	0.00275178528267
100.0	1.025	1.025	-76.17842019347876	0.00274425945614
110.0	1.025	1.025	-76.17684032453977	0.00273627405714
120.0	1.025	1.025	-76.17085479450560	0.00272741447159
130.0	1.025	1.025	-76.16140688347379	0.00271772066960
140.0	1.025	1.025	-76.14968739859238	0.00270749976121
80.0	1.025	1.075	-76.16064659384156	0.00275982994397

100.0	1.025	1.075	-76.17239768793340	0.00274439522091
110.0	1.025	1.075	-76.17038824344327	0.00273689691931
120.0	1.025	1.075	-76.16405085994603	0.00272878137167
130.0	1.025	1.075	-76.15427766338800	0.00272007909736
140.0	1.025	1.075	-76.14220750764144	0.00271106111475
80.0	1.075	1.075	-76.15582697760905	0.00275954955289
90.0	1.075	1.075	-76.16388141833413	0.00275144743205
100.0	1.075	1.075	-76.16642710450151	0.00274445096450
110.0	1.075	1.075	-76.16403230131576	0.00273749098487
120.0	1.075	1.075	-76.15737961246926	0.00273018676612
130.0	1.075	1.075	-76.14731097717730	0.00272256947817
100.0	0.825	1.125	-76.14082883341572	0.00276507103173
110.0	0.825	1.125	-76.13986382866057	0.00275638755416
80.0	0.875	1.125	-76.14386499233557	0.00277290644287
90.0	0.875	1.125	-76.15360352445157	0.00276462565167
100.0	0.875	1.125	-76.15746909319139	0.00275686084581
110.0	0.875	1.125	-76.15613791107390	0.00274857152555
120.0	0.875	1.125	-76.15039133728520	0.00273936546009
130.0	0.875	1.125	-76.14118185018197	0.00272934559117
90.0	0.875	1.175	-76.14452277953419	0.00276777123650
100.0	0.875	1.175	-76.14772110547796	0.00276023583306
110.0	0.875	1.175	-76.14588002131363	0.00275250045117
120.0	0.875	1.175	-76.13972727565779	0.00274418400358
70.0	0.925	0.925	-76.14252257499258	0.00277806119157
70.0	0.925	0.975	-76.14668457648104	0.00277569583067
70.0	0.925	1.025	-76.14638335899252	0.00277502624315
70.0	0.925	1.075	-76.14291361498556	0.00277581892324
80.0	0.925	1.125	-76.15278735998945	0.00276692123507
90.0	0.925	1.125	-76.16195892156682	0.00275869865336
100.0	0.925	1.125	-76.16537440914925	0.00275118025797
110.0	0.925	1.125	-76.16367561063319	0.00274330635776
120.0	0.925	1.125	-76.15761356451053	0.00273467940253
130.0	0.925	1.125	-76.14810743311304	0.00272536700361
80.0	0.925	1.175	-76.14452219605923	0.00276987718062
90.0	0.925	1.175	-76.15288002723717	0.00276163294680
100.0	0.925	1.175	-76.15567902130020	0.00275440915986
110.0	0.925	1.175	-76.15351252730156	0.00274715215491
120.0	0.925	1.175	-76.14707940766995	0.00273948850426
90.0	0.925	1.225	-76.14289462734681	0.00276585923944
100.0	0.925	1.225	-76.14510760156401	0.00275904315114
110.0	0.925	1.225	-76.14250717293189	0.00275257237208
70.0	0.975	0.975	-76.15064548516331	0.00277300183669
70.0	0.975	1.025	-76.15015838225585	0.00277202064800
70.0	0.975	1.075	-76.14651947568584	0.00277250214434
70.0	0.975	1.125	-76.14068359143526	0.00277427560912
80.0	0.975	1.125	-76.15547426577334	0.00276309404208
90.0	0.975	1.125	-76.16406375300954	0.00275492272944
100.0	0.975	1.125	-76.16702474285975	0.00274766130827
110.0	0.975	1.125	-76.16496193174558	0.00274024264495
120.0	0.975	1.125	-76.15859185822995	0.00273227290788
130.0	0.975	1.125	-76.14879468804435	0.00272379917422
80.0	0.975	1.175	-76.14715011254641	0.00276580011878
90.0	0.975	1.175	-76.15498785635984	0.00275767820043
100.0	0.975	1.175	-76.15738299029566	0.00275076750643
110.0	0.975	1.175	-76.15489460816198	0.00274402077116
120.0	0.975	1.175	-76.14818853114900	0.00273708309066
90.0	0.975	1.225	-76.14501129388479	0.00276170207861
100.0	0.975	1.225	-76.14686798678638	0.00275525024801
110.0	0.975	1.225	-76.14398544355328	0.00274934000055
70.0	1.025	1.025	-76.14949729506452	0.00277075061392
70.0	1.025	1.075	-76.14569825230743	0.00277095154591
80.0	1.025	1.125	-76.15372138221078	0.00276108177231
90.0	1.025	1.125	-76.16172123454204	0.00275297801441
100.0	1.025	1.125	-76.16422887500570	0.00274600375991
110.0	1.025	1.125	-76.16181034508698	0.00273909617658
120.0	1.025	1.125	-76.15514405888365	0.00273188128600

80.0	1.025	1.175	-76.14534164870629	0.00276357074810
90.0	1.025	1.175	-76.15265073193312	0.00275557809431
100.0	1.025	1.175	-76.15464248681704	0.00274900166415
110.0	1.025	1.175	-76.15183996921076	0.00274281393733
120.0	1.025	1.175	-76.14487243610682	0.00273669370174
90.0	1.025	1.225	-76.14268480462333	0.00275942411112
100.0	1.025	1.225	-76.14418533481789	0.00275334909673
110.0	1.025	1.225	-76.14102809545396	0.00274804011845
70.0	1.075	1.075	-76.14175025021163	0.00277088572299
80.0	1.075	1.125	-76.14884283362277	0.00276061484504
90.0	1.075	1.125	-76.15625237084714	0.00275261343780
100.0	1.075	1.125	-76.15831307059045	0.00274597306179
110.0	1.075	1.125	-76.15555171236244	0.00273964996446
120.0	1.075	1.125	-76.14860553189919	0.00273330935859
90.0	1.075	1.175	-76.14719040710929	0.00275507278610
100.0	1.075	1.175	-76.14878407364236	0.00274886876690
110.0	1.075	1.175	-76.14567940867256	0.00274330677196
80.0	1.125	1.125	-76.14180641271703	0.00276150106002
90.0	1.125	1.125	-76.14863113017084	0.00275365530881
100.0	1.125	1.125	-76.15025625417027	0.00274740368443
110.0	1.125	1.125	-76.14716944860761	0.00274175391396

Table IIS: The fit to the CASSCF BODC (in atomic units).

rtilde=1.795239689149971 xtilde= -0.25

i	j	k	Cijk
0	0	0	2.74600811383720E-03
0	0	1	5.27778953307003E-05
0	0	2	-3.11961244906481E-05
0	0	3	3.06298678489347E-05
0	0	4	7.86378521145456E-06
0	0	5	1.31018215121837E-05
0	0	6	-1.06753486859016E-05
0	0	7	2.48741800302526E-05
0	0	8	2.52545413869764E-05
0	1	0	-3.26966914293352E-05
0	1	1	-1.44660947327592E-05
0	1	2	3.54549315928144E-05
0	1	3	-1.65827290273285E-06
0	1	4	1.51091084574955E-05
0	1	5	2.58257011337831E-05
0	1	6	-1.50575161856886E-05
0	1	7	-2.24700976091234E-05
0	2	0	1.10453049929606E-04
0	2	1	-2.09733016729192E-05
0	2	2	2.77305878781581E-05
0	2	3	-3.28870046626335E-05
0	2	4	1.06408226739248E-05
0	2	5	-2.34169820017061E-05
0	2	6	7.51858522584816E-05
0	3	0	-5.15264814823363E-05
0	3	1	-1.79454620936696E-05
0	3	2	9.10303639750682E-06
0	3	3	-1.21656322595770E-05
0	3	4	9.68239927898854E-06
0	3	5	-7.82667128305949E-05
0	4	0	3.17225912126714E-05
0	4	1	1.56500653546223E-06
0	4	2	2.38836039324041E-05
0	4	3	-5.19708954787017E-07
0	4	4	4.58531504166844E-05
0	5	0	1.48618241401931E-06
0	5	1	5.69319652187645E-06
0	5	2	3.98901276042152E-05
0	5	3	-3.11287156926382E-05
0	6	0	2.28000066981285E-05
0	6	1	-8.42433297150545E-05
0	6	2	-5.10853359637589E-05
0	7	0	-2.61396184121282E-05
0	7	1	8.64602011403562E-05
0	8	0	-1.31006897871585E-05
1	0	0	-3.26966914292907E-05
1	0	1	-1.44660947327142E-05
1	0	2	3.54549315926157E-05
1	0	3	-1.65827290498402E-06
1	0	4	1.51091084596409E-05
1	0	5	2.58257011469398E-05
1	0	6	-1.50575161918176E-05
1	0	7	-2.24700976301859E-05
1	1	0	-7.60801783855523E-06
1	1	1	-4.32841051855291E-05
1	1	2	1.25917683446481E-05
1	1	3	-5.30021867058902E-05
1	1	4	2.74574230960380E-06
1	1	5	1.57961011920048E-05
1	1	6	4.79265243783921E-05
1	2	0	5.92761678480573E-06
1	2	1	1.15867365725195E-05

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1 2 3 -2.70126314403687E-06
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